



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:02 am GMT

PDB ID : 3DP8  
Title : Structural characterization of a putative endogenous metal chelator in the periplasmic nickel transporter NikA (nickel butane-1,2,4-tricarboxylate form)  
Authors : Cherrier, M.V.; Cavazza, C.; Bochot, C.; Lemaire, D.; Fontecilla-Camps, J.C.  
Deposited on : 2008-07-07  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

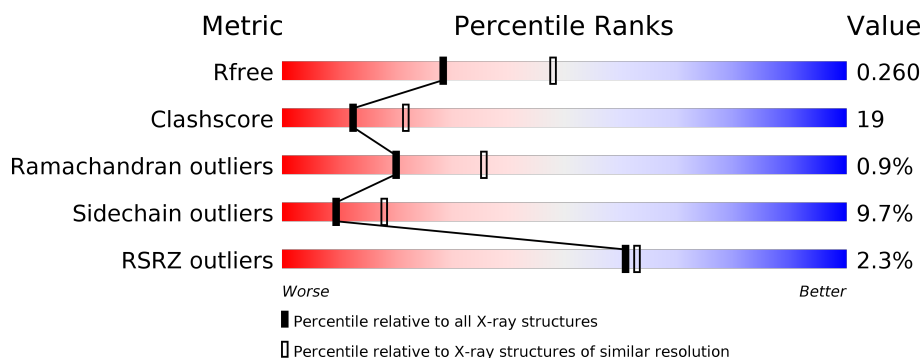
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	502	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 67%; height: 10px; background-color: green;"></div> <div style="width: 27%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>67%</span> <span>27%</span> <span>5%</span> <span>1%</span> </div> </div>
1	B	502	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 69%; height: 10px; background-color: green;"></div> <div style="width: 24%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>69%</span> <span>24%</span> <span>5%</span> <span>1%</span> </div> </div>
1	C	502	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">5%</span> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 64%; height: 10px; background-color: green;"></div> <div style="width: 30%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: red;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>64%</span> <span>30%</span> <span>5%</span> <span>1%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	504	-	-	-	X
3	ACT	A	506	-	-	X	X
3	ACT	A	507	-	-	X	X
3	ACT	B	504	-	-	-	X
3	ACT	B	506	-	-	-	X
3	ACT	B	507	-	-	X	X
3	ACT	C	504	-	-	X	X
3	ACT	C	506	-	-	X	X
7	GOL	A	512	-	-	-	X
7	GOL	A	513	-	-	X	-
7	GOL	A	514	-	-	X	X
7	GOL	A	515	-	-	-	X
7	GOL	B	513	-	-	X	X
7	GOL	B	515	-	-	X	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12491 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nickel-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	15	0
			4019	2582	672	755	10			
1	B	497	Total	C	N	O	S	6	18	0
			4055	2609	680	755	11			
1	C	496	Total	C	N	O	S	0	11	0
			4006	2570	673	751	12			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		
2	C	1	Total	Ni	0	0
			1	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

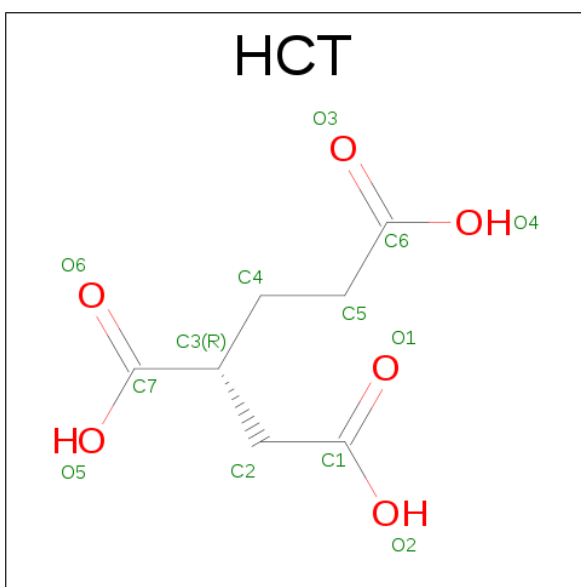


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

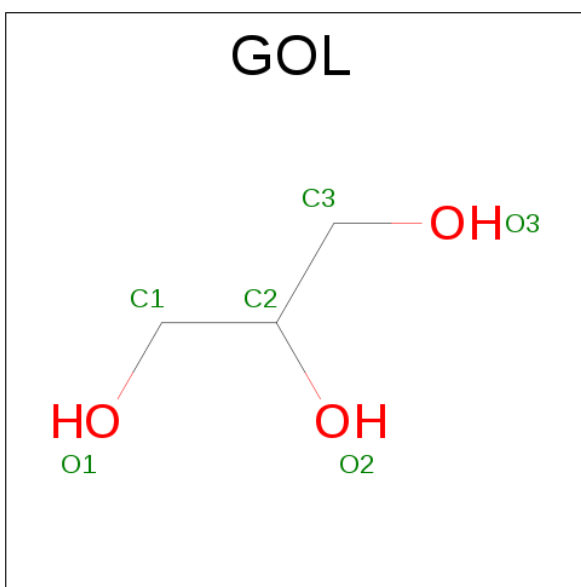
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Cl	0	0
			3	3		
5	A	2	Total	Cl	0	0
			2	2		
5	C	2	Total	Cl	0	0
			2	2		

- Molecule 6 is (2R)-BUTANE-1,2,4-TRICARBOXYLIC ACID (three-letter code: HCT) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	7	6		
6	B	1	Total	C	O	0	0
			13	7	6		
6	C	1	Total	C	O	0	0
			13	7	6		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0

- Molecule 8 is water.

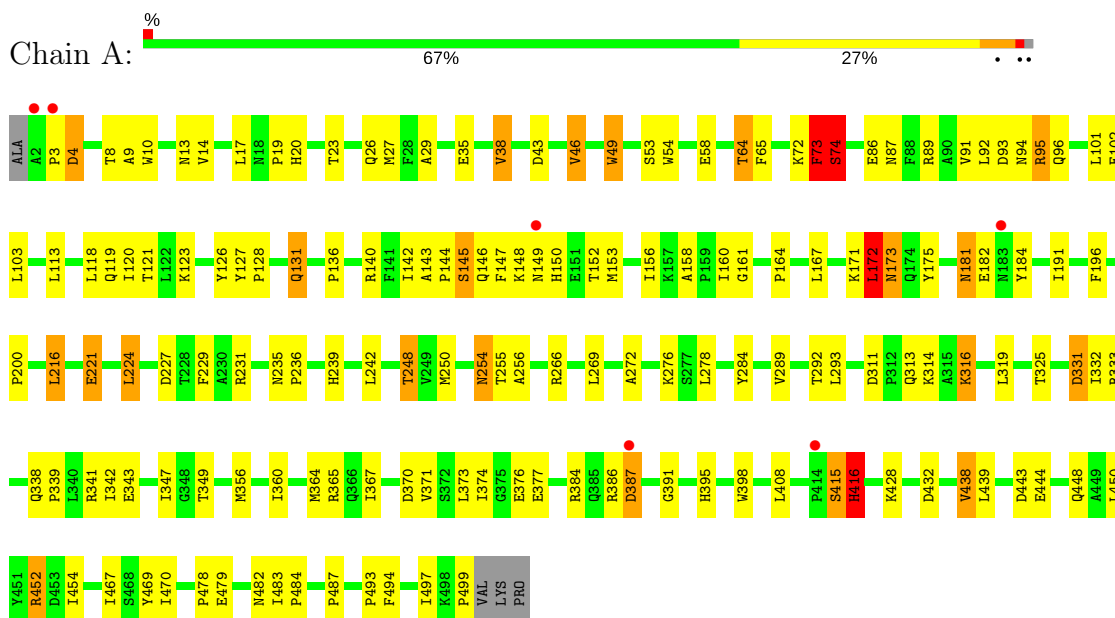
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	100	Total 100	O 100	0	0
8	B	110	Total 110	O 110	0	0
8	C	55	Total 55	O 55	0	0



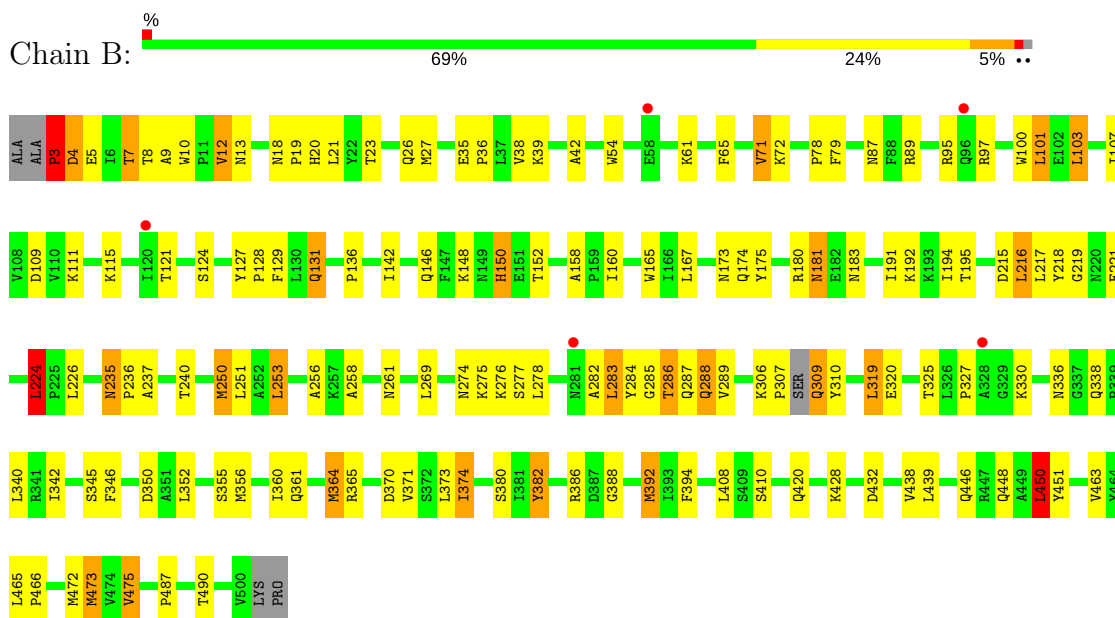
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

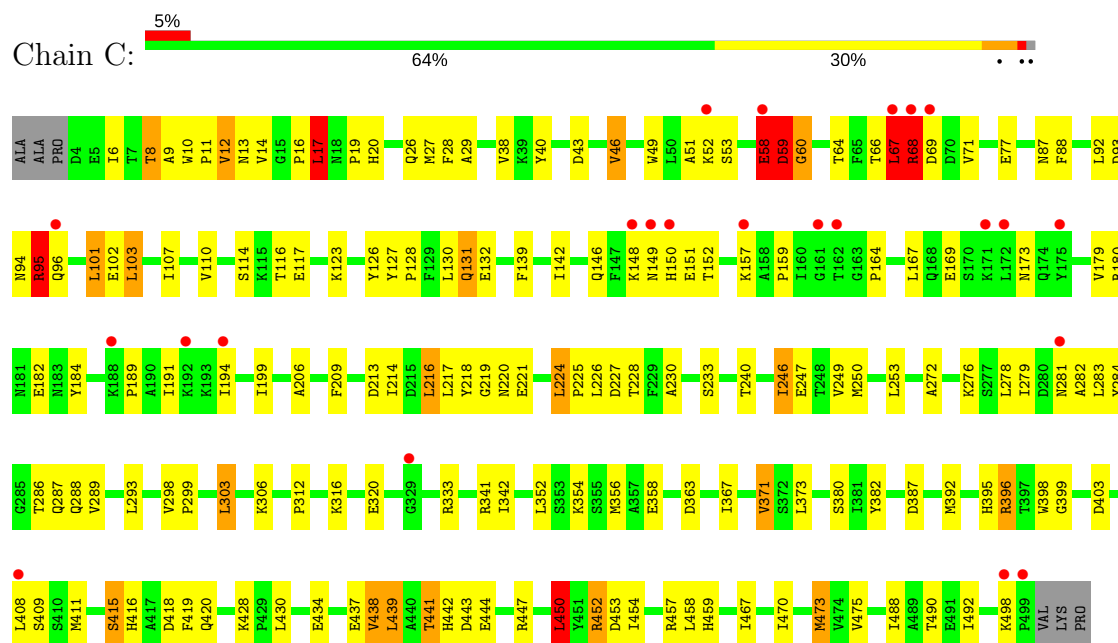
#### • Molecule 1: Nickel-binding periplasmic protein



#### • Molecule 1: Nickel-binding periplasmic protein



● Molecule 1: Nickel-binding periplasmic protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.57Å 158.57Å 134.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-2.50) 99.7 (19.91-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.20 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.199 , 0.270 0.194 , 0.260	Depositor DCC
$R_{free}$ test set	1707 reflections (2.64%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.2	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12491	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, HCT, NI, CL, SO4, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.92	1/4167 (0.0%)	0.94	8/5676 (0.1%)
1	B	0.91	1/4212 (0.0%)	0.96	7/5729 (0.1%)
1	C	0.82	0/4139	0.85	6/5634 (0.1%)
All	All	0.88	2/12518 (0.0%)	0.92	21/17039 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	4
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	TRP	CB-CG	5.62	1.60	1.50
1	B	382	TYR	CB-CG	5.38	1.59	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	LEU	CA-CB-CG	9.06	136.15	115.30
1	A	452	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	231	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	A	73	PHE	N-CA-C	-7.51	90.73	111.00
1	B	4	ASP	N-CA-C	7.33	130.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	ARG	CG-CD-NE	-6.80	97.52	111.80
1	C	303	LEU	CA-CB-CG	6.07	129.27	115.30
1	C	450	LEU	CA-CB-CG	5.88	128.83	115.30
1	A	416	HIS	N-CA-CB	5.77	120.99	110.60
1	C	452	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	3	PRO	C-N-CA	5.52	135.49	121.70
1	A	231	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	450	LEU	CA-CB-CG	5.41	127.74	115.30
1	B	475	VAL	CG1-CB-CG2	-5.40	102.27	110.90
1	C	68	ARG	CB-CA-C	5.37	121.14	110.40
1	C	60	GLY	N-CA-C	-5.33	99.77	113.10
1	A	74	SER	N-CA-CB	5.29	118.44	110.50
1	B	319	LEU	CB-CG-CD1	5.29	120.00	111.00
1	C	452	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	370	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	443	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	LEU	Peptide
1	A	415	SER	Peptide
1	A	73	PHE	Peptide
1	B	215	ASP	Peptide
1	B	3	PRO	Peptide
1	B	309[B]	GLN	Mainchain
1	C	58	GLU	Peptide
1	C	59	ASP	Peptide
1	C	67	LEU	Peptide
1	C	68	ARG	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4019	0	4002	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4055	0	4060	154	0
1	C	4006	0	3975	164	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	16	0	12	5	0
3	B	16	0	12	16	0
3	C	12	0	9	18	0
4	A	5	0	0	0	0
5	A	2	0	0	0	0
5	B	3	0	0	1	0
5	C	2	0	0	0	0
6	A	13	0	6	1	0
6	B	13	0	7	0	0
6	C	13	0	6	0	0
7	A	24	0	32	15	0
7	B	24	0	32	9	0
8	A	100	0	0	14	0
8	B	110	0	0	12	0
8	C	55	0	0	5	0
All	All	12491	0	12153	455	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (455) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396[A]:ARG:NH2	3:C:506:ACT:CH3	1.97	1.27
1:A:377[A]:GLU:HA	7:A:513:GOL:O1	1.33	1.26
1:C:396[A]:ARG:NH2	3:C:506:ACT:H2	1.52	1.21
1:A:377[B]:GLU:HA	7:A:513:GOL:O1	1.48	1.13
1:A:95:ARG:HH11	1:A:95:ARG:HG3	1.09	1.11
1:C:67:LEU:HB3	1:C:68:ARG:HB2	1.35	1.08
1:A:4:ASP:HA	8:A:607:HOH:O	1.53	1.07
1:A:356:MET:HE1	1:A:467:ILE:HG21	1.32	1.06
1:C:396[A]:ARG:CG	3:C:506:ACT:H3	1.87	1.04
1:A:92:LEU:HD22	1:A:95:ARG:HH12	1.23	1.03
1:A:38:VAL:HG13	1:A:46:VAL:HG21	1.40	1.00
1:C:396[A]:ARG:HG3	3:C:506:ACT:H3	1.43	0.98
1:A:316:LYS:HE2	1:A:333:ARG:HH11	1.27	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ALA:H	3:B:507:ACT:H3	1.26	0.98
1:A:95:ARG:HH11	1:A:95:ARG:CG	1.76	0.97
1:A:13:ASN:HD21	1:A:173:ASN:HA	1.27	0.95
1:C:226:LEU:HD21	1:C:473[B]:MET:HE3	1.44	0.95
1:B:217:LEU:HD23	3:B:507:ACT:H1	1.47	0.95
1:C:396[A]:ARG:HH21	3:C:506:ACT:CH3	1.78	0.91
1:A:35[B]:GLU:HG2	1:A:49:TRP:HE1	1.33	0.91
1:C:283:LEU:HD13	1:C:287[B]:GLN:OE1	1.69	0.91
1:A:95:ARG:HG3	1:A:95:ARG:NH1	1.81	0.90
1:C:396[A]:ARG:HG3	3:C:506:ACT:CH3	2.01	0.89
1:B:8:THR:OG1	3:B:507:ACT:CH3	2.20	0.89
1:A:14[B]:VAL:CG2	1:A:29:ALA:CB	2.50	0.88
1:C:58:GLU:OE1	1:C:58:GLU:HA	1.73	0.87
1:B:388:GLY:HA3	7:B:513:GOL:H11	1.54	0.87
7:A:514:GOL:H31	1:B:42:ALA:H	1.40	0.86
1:B:274:ASN:OD1	1:B:277:SER:HB3	1.75	0.86
1:A:239:HIS:HB2	1:B:448:GLN:HE22	1.41	0.86
1:C:396[A]:ARG:NH2	3:C:506:ACT:H3	1.92	0.85
1:C:226:LEU:HD21	1:C:473[B]:MET:CE	2.07	0.84
1:A:248:THR:HG21	1:A:293:LEU:O	1.78	0.84
1:B:217:LEU:HD23	3:B:507:ACT:CH3	2.08	0.83
1:B:285:GLY:HA2	1:B:286:THR:OG1	1.77	0.83
1:C:396[A]:ARG:CZ	3:C:506:ACT:CH3	2.57	0.82
1:B:364:MET:SD	8:B:620:HOH:O	2.38	0.81
1:A:152[B]:THR:HG23	1:A:156:ILE:HG23	1.63	0.81
1:A:313:GLN:HG2	8:A:604:HOH:O	1.81	0.81
1:A:38:VAL:HG13	1:A:46:VAL:CG2	2.11	0.81
1:B:269[B]:LEU:HD13	1:B:364:MET:SD	2.22	0.80
1:C:13:ASN:ND2	1:C:173:ASN:H	1.79	0.80
1:B:8:THR:OG1	3:B:507:ACT:H2	1.82	0.79
1:A:92:LEU:HD22	1:A:95:ARG:NH1	1.97	0.79
1:C:38:VAL:HG22	1:C:46:VAL:HG13	1.65	0.78
1:B:9:ALA:H	3:B:507:ACT:CH3	1.97	0.78
1:C:396[A]:ARG:CD	3:C:506:ACT:H3	2.12	0.78
7:A:514:GOL:H12	1:B:42:ALA:HB2	1.66	0.78
1:A:377[A]:GLU:CA	7:A:513:GOL:O1	2.25	0.78
1:C:13:ASN:HD21	1:C:173:ASN:H	1.29	0.78
1:C:442:HIS:HD2	8:C:563:HOH:O	1.66	0.78
1:B:146:GLN:HE21	1:B:158:ALA:H	1.31	0.77
1:B:269[B]:LEU:HD21	1:B:392:MET:SD	2.26	0.76
1:B:256:ALA:HB3	7:B:513:GOL:H32	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:VAL:HA	1:C:450:LEU:HD23	1.66	0.76
1:A:8:THR:HG22	1:A:9:ALA:H	1.50	0.75
1:B:97[B]:ARG:HH11	1:B:386:ARG:NH1	1.84	0.75
1:A:14[B]:VAL:CG2	1:A:29:ALA:HB2	2.16	0.75
1:B:95:ARG:NH2	1:B:107:ILE:O	2.19	0.75
1:C:226:LEU:CD2	1:C:473[B]:MET:CE	2.64	0.74
1:A:14[B]:VAL:HG21	1:A:29:ALA:CB	2.16	0.74
7:A:514:GOL:C3	1:B:42:ALA:H	2.00	0.74
3:A:506:ACT:C	1:B:288[B]:GLN:HE22	2.01	0.73
1:C:226:LEU:CD2	1:C:473[B]:MET:HE1	2.19	0.72
1:A:27:MET:HG3	8:A:535:HOH:O	1.89	0.72
1:B:10:TRP:HE1	1:B:26:GLN:HE21	1.36	0.71
1:B:221:GLU:HG2	1:B:473[B]:MET:HE3	1.71	0.71
1:A:356:MET:CE	1:A:467:ILE:HG21	2.17	0.71
1:A:313:GLN:CG	8:A:604:HOH:O	2.37	0.71
1:C:58:GLU:N	1:C:59:ASP:HB2	2.05	0.71
1:B:217:LEU:CD2	3:B:507:ACT:H1	2.19	0.71
1:A:152[B]:THR:HG23	1:A:156:ILE:CG2	2.21	0.70
1:C:10:TRP:HE1	1:C:26:GLN:HE21	1.38	0.70
1:C:286:THR:O	1:C:287[A]:GLN:NE2	2.23	0.70
1:B:438:VAL:HG13	1:B:450:LEU:HB3	1.71	0.70
1:B:276[B]:LYS:HE3	8:B:589:HOH:O	1.90	0.70
1:C:13:ASN:HD21	1:C:173:ASN:N	1.89	0.70
1:C:316:LYS:HG3	1:C:367[A]:ILE:HD13	1.73	0.69
1:A:314[B]:LYS:HE3	8:A:594:HOH:O	1.93	0.69
1:C:226:LEU:HD12	1:C:283:LEU:HD23	1.74	0.69
1:B:8:THR:OG1	3:B:507:ACT:H3	1.93	0.69
1:C:38:VAL:CG2	1:C:46:VAL:HG13	2.23	0.68
1:C:67:LEU:HB3	1:C:68:ARG:CB	2.17	0.68
1:B:20:HIS:HD2	1:B:152:THR:OG1	1.76	0.68
1:A:272:ALA:HB2	1:A:367:ILE:HD13	1.76	0.68
1:A:254:ASN:HD22	1:A:256:ALA:H	1.39	0.68
1:A:316:LYS:CE	1:A:333:ARG:HH11	2.03	0.68
1:A:35[B]:GLU:HG2	1:A:49:TRP:NE1	2.06	0.66
1:B:216:LEU:O	3:B:507:ACT:H2	1.96	0.66
1:B:253:LEU:HD12	1:B:392:MET:HG3	1.77	0.66
1:A:14[A]:VAL:HG13	1:A:29:ALA:CB	2.26	0.66
1:B:23:THR:HG21	1:B:382:TYR:CD2	2.31	0.66
1:C:68:ARG:HB3	1:C:69:ASP:HA	1.77	0.66
1:B:276[A]:LYS:HE3	8:B:589:HOH:O	1.97	0.65
1:B:288[A]:GLN:HE21	1:B:288[A]:GLN:H	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:VAL:CG1	1:B:450:LEU:HB3	2.26	0.65
1:A:13:ASN:ND2	1:A:173:ASN:HA	2.07	0.65
1:C:52:LYS:HG3	1:C:68:ARG:H	1.61	0.65
1:A:64:THR:HG23	1:A:119:GLN:HG3	1.79	0.65
1:B:142:ILE:HG13	1:B:160:ILE:O	1.97	0.65
1:B:251:LEU:HD13	1:B:392:MET:HG2	1.78	0.65
1:B:7:THR:HB	1:B:195:THR:HB	1.78	0.64
1:B:278:LEU:O	1:B:282:ALA:HB3	1.98	0.64
1:C:396[A]:ARG:HH21	3:C:506:ACT:H3	1.52	0.64
1:B:342:ILE:O	1:B:371:VAL:HA	1.98	0.64
1:B:269[B]:LEU:CD1	1:B:364:MET:SD	2.87	0.63
1:B:226:LEU:CD1	1:B:283:LEU:HA	2.29	0.63
1:B:250:MET:HB2	1:B:466:PRO:HA	1.80	0.63
1:C:226:LEU:HD23	1:C:473[B]:MET:HE1	1.80	0.63
1:A:131[A]:GLN:NE2	1:A:131[A]:GLN:H	1.97	0.63
1:A:14[A]:VAL:HG12	1:A:17:LEU:HD13	1.80	0.62
1:B:446[A]:GLN:HG3	1:B:450:LEU:HD22	1.80	0.62
1:B:103:LEU:HD21	1:B:129:PHE:CD2	2.35	0.62
1:B:217:LEU:HD13	1:B:224:LEU:HD22	1.82	0.62
1:A:14[B]:VAL:HG23	1:A:29:ALA:HB2	1.81	0.62
1:B:180:ARG:NH2	1:B:192[B]:LYS:HE2	2.15	0.62
1:A:92:LEU:CD2	1:A:95:ARG:HH12	2.07	0.62
1:B:283:LEU:HD21	1:B:352:LEU:HD11	1.81	0.62
7:A:514:GOL:H12	1:B:42:ALA:CB	2.30	0.62
1:C:382:TYR:HE2	1:C:416:HIS:CE1	2.16	0.62
1:B:180:ARG:HH22	1:B:192[B]:LYS:HE2	1.63	0.61
1:C:180:ARG:HD2	1:C:189:PRO:HD2	1.82	0.61
1:C:396[A]:ARG:HH21	3:C:506:ACT:H2	1.41	0.61
1:C:293:LEU:HB3	3:C:504:ACT:H3	1.82	0.61
1:B:9:ALA:N	3:B:507:ACT:H3	2.07	0.61
1:C:103:LEU:HD13	1:C:139:PHE:CE1	2.34	0.61
1:B:127:TYR:CG	1:B:128:PRO:HD3	2.36	0.61
1:B:276[A]:LYS:CE	8:B:589:HOH:O	2.48	0.61
1:C:217:LEU:HD13	1:C:224:LEU:HD22	1.82	0.61
1:C:287[A]:GLN:HG3	1:C:470:ILE:HA	1.83	0.61
1:B:18:ASN:ND2	1:B:21:LEU:HD23	2.16	0.60
1:C:442:HIS:CD2	8:C:563:HOH:O	2.47	0.60
1:C:114:SER:HB3	1:C:117:GLU:HB2	1.83	0.60
1:C:10:TRP:HE1	1:C:26:GLN:NE2	1.99	0.60
1:A:14[B]:VAL:HG21	1:A:29:ALA:HB1	1.82	0.60
1:B:364:MET:HG3	1:B:371:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LYS:HE2	8:B:586:HOH:O	2.01	0.60
1:C:283:LEU:CD2	1:C:352:LEU:CD1	2.79	0.60
1:B:103:LEU:HD21	1:B:129:PHE:HD2	1.67	0.60
1:A:316:LYS:HE3	1:A:367:ILE:HA	1.84	0.60
1:A:4:ASP:N	1:A:4:ASP:OD2	2.35	0.60
1:A:364:MET:HG3	1:A:371:VAL:HG11	1.84	0.60
1:A:20:HIS:HE1	1:A:140:ARG:O	1.85	0.59
1:A:331:ASP:HB3	1:A:365:ARG:HH11	1.67	0.59
1:B:278:LEU:HD21	1:B:356:MET:HG2	1.83	0.59
1:A:254:ASN:ND2	1:A:256:ALA:H	2.00	0.59
1:A:102:GLU:HB3	1:A:126:TYR:OH	2.03	0.58
1:A:248:THR:HB	1:A:469:TYR:CD1	2.37	0.58
1:A:3:PRO:HA	8:A:607:HOH:O	2.02	0.58
1:A:470:ILE:HD12	1:A:470:ILE:C	2.24	0.58
1:B:8:THR:HG1	3:B:507:ACT:H2	1.67	0.58
1:C:420:GLN:HA	1:C:420:GLN:HE21	1.68	0.58
1:B:146:GLN:NE2	1:B:158:ALA:H	2.00	0.58
1:B:283:LEU:HD12	1:B:287:GLN:HG3	1.84	0.58
1:B:288[A]:GLN:NE2	1:B:288[A]:GLN:H	2.02	0.57
1:A:13:ASN:HD21	1:A:172:LEU:HA	1.68	0.57
1:B:388:GLY:HA3	7:B:513:GOL:C1	2.32	0.57
1:B:23:THR:HG21	1:B:382:TYR:HD2	1.67	0.57
1:B:420:GLN:NE2	7:B:513:GOL:O3	2.37	0.57
1:C:219:GLY:O	1:C:473[A]:MET:HG3	2.04	0.57
1:C:88:PHE:HB3	1:C:110:VAL:HG21	1.86	0.57
1:B:428:LYS:NZ	1:B:432:ASP:OD1	2.34	0.57
1:B:61:LYS:HD3	1:B:124:SER:HA	1.86	0.57
1:B:109:ASP:HB3	1:B:121:THR:OG1	2.05	0.57
1:B:10:TRP:HE1	1:B:26:GLN:NE2	2.02	0.57
1:C:126:TYR:CZ	1:C:128:PRO:HG2	2.40	0.56
1:A:248:THR:HB	1:A:469:TYR:HD1	1.70	0.56
1:B:235:ASN:C	1:B:235:ASN:HD22	2.08	0.56
1:C:283:LEU:HD21	1:C:352:LEU:CD1	2.35	0.56
1:C:68:ARG:HB3	1:C:69:ASP:CA	2.35	0.56
1:A:278:LEU:HD21	1:A:356:MET:HG2	1.86	0.56
1:C:438:VAL:CA	1:C:450:LEU:HD23	2.34	0.56
1:B:373:LEU:HD22	7:B:515:GOL:C3	2.34	0.56
1:C:396[A]:ARG:HH22	3:C:506:ACT:H2	1.59	0.56
1:A:494:PHE:HA	1:A:497:ILE:HD12	1.88	0.56
1:C:430:LEU:C	1:C:430:LEU:HD23	2.26	0.56
1:A:43:ASP:HB3	7:A:514:GOL:H2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:PHE:HB3	1:B:394:PHE:CD1	2.41	0.56
1:C:246:ILE:H	1:C:246:ILE:HD13	1.71	0.56
1:C:221:GLU:OE1	1:C:287[A]:GLN:NE2	2.39	0.56
1:A:136:PRO:O	1:A:140:ARG:HD2	2.05	0.56
1:B:219:GLY:CA	1:B:472:MET:CE	2.84	0.56
1:C:288[B]:GLN:CD	1:C:289:VAL:H	2.09	0.56
1:C:59:ASP:HB3	1:C:60:GLY:HA2	1.88	0.56
1:A:428:LYS:HE3	1:A:432:ASP:OD2	2.06	0.55
1:A:87:ASN:HD21	1:A:142:ILE:H	1.54	0.55
1:C:95:ARG:NH2	1:C:107:ILE:O	2.39	0.55
1:B:327:PRO:HG2	1:B:330:LYS:HB2	1.87	0.55
1:A:311:ASP:CG	1:A:314[B]:LYS:HG3	2.27	0.55
1:A:332:ILE:HD13	1:A:370:ASP:HB2	1.88	0.55
1:B:3:PRO:N	1:B:5:GLU:H	2.04	0.55
1:A:153:MET:HG2	8:A:578:HOH:O	2.07	0.55
1:B:235:ASN:ND2	1:B:237:ALA:H	2.05	0.55
1:C:149:ASN:O	1:C:150:HIS:HB2	2.06	0.55
1:A:10:TRP:HE1	1:A:26:GLN:NE2	2.05	0.55
1:A:148:LYS:O	1:A:149:ASN:HB2	2.07	0.55
1:B:219:GLY:HA2	1:B:472:MET:CE	2.37	0.55
1:B:87:ASN:HD21	1:B:142:ILE:HG22	1.72	0.54
1:B:274:ASN:HB2	1:B:310:TYR:CE1	2.42	0.54
1:A:276:LYS:HE2	7:A:512:GOL:O1	2.07	0.54
7:A:514:GOL:H31	1:B:42:ALA:CB	2.37	0.54
7:A:514:GOL:H32	1:B:487:PRO:HG3	1.88	0.54
1:B:13:ASN:HD21	1:B:173:ASN:H	1.56	0.54
1:C:396[A]:ARG:CZ	3:C:506:ACT:H3	2.31	0.54
1:A:73:PHE:CE2	1:A:143:ALA:N	2.75	0.54
1:C:38:VAL:CG2	1:C:46:VAL:CG1	2.86	0.54
1:B:338:GLN:HE21	1:C:430:LEU:HB2	1.73	0.54
1:A:87:ASN:HD21	1:A:142:ILE:HG22	1.72	0.54
1:A:87:ASN:O	1:A:91:VAL:HG23	2.08	0.54
1:B:373:LEU:HD22	7:B:515:GOL:H32	1.89	0.54
1:C:114:SER:HB3	1:C:117:GLU:CB	2.38	0.53
1:A:38:VAL:CG1	1:A:46:VAL:HG21	2.27	0.53
1:A:487:PRO:HD2	8:A:525:HOH:O	2.08	0.53
1:B:360:ILE:O	1:B:364:MET:HG2	2.08	0.53
1:A:19:PRO:HG3	1:A:142:ILE:HB	1.89	0.53
1:C:38:VAL:HG22	1:C:46:VAL:CG1	2.38	0.53
1:C:437:GLU:O	1:C:441:THR:HG22	2.08	0.53
1:C:382:TYR:HE2	1:C:416:HIS:HE1	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:MET:HE1	1:A:467:ILE:CG2	2.23	0.53
1:A:8:THR:HG23	1:A:216:LEU:O	2.08	0.53
1:B:278:LEU:C	1:B:278:LEU:HD23	2.29	0.53
1:C:415:SER:HA	8:C:547:HOH:O	2.09	0.52
1:B:250:MET:CB	1:B:466:PRO:HA	2.40	0.52
1:B:148:LYS:O	5:B:510:CL:CL	2.64	0.52
1:B:71:VAL:HG22	1:B:79:PHE:HB3	1.90	0.52
1:A:269:LEU:HD22	1:A:364:MET:HE3	1.91	0.52
1:B:276[B]:LYS:CE	8:B:589:HOH:O	2.53	0.52
1:B:226:LEU:HD13	1:B:283:LEU:HA	1.91	0.52
1:C:19:PRO:HG3	1:C:142:ILE:HB	1.91	0.52
1:A:200:PRO:HG2	8:A:597:HOH:O	2.09	0.52
1:A:360:ILE:O	1:A:364:MET:HG2	2.09	0.52
1:A:72:LYS:C	1:A:73:PHE:O	2.41	0.52
1:A:43:ASP:HB3	7:A:514:GOL:C2	2.39	0.52
1:B:18:ASN:ND2	1:B:21:LEU:CD2	2.73	0.52
1:C:246:ILE:HG12	1:C:247:GLU:HG2	1.90	0.52
1:A:444:GLU:O	1:A:448:GLN:HG3	2.10	0.52
1:A:131[A]:GLN:CD	1:A:131[A]:GLN:H	2.12	0.51
1:C:87:ASN:HD21	1:C:142:ILE:HG22	1.74	0.51
1:A:127:TYR:CD2	1:A:128:PRO:HD3	2.45	0.51
1:A:248:THR:HG22	8:A:521:HOH:O	2.10	0.51
1:B:446[A]:GLN:HG2	8:B:623:HOH:O	2.10	0.51
1:B:13:ASN:HD21	1:B:173:ASN:N	2.07	0.51
1:C:10:TRP:CG	1:C:11:PRO:HD2	2.45	0.51
1:C:246:ILE:HD13	1:C:470:ILE:O	2.09	0.51
1:C:49:TRP:C	1:C:51:ALA:N	2.64	0.51
1:C:443:ASP:C	1:C:443:ASP:OD1	2.49	0.51
1:C:230:ALA:O	1:C:233:SER:HB2	2.11	0.51
1:C:286:THR:O	1:C:287[A]:GLN:CD	2.49	0.51
1:C:312:PRO:O	1:C:367[A]:ILE:HD11	2.11	0.51
1:C:281:ASN:O	1:C:283:LEU:N	2.44	0.51
1:C:316:LYS:HE2	8:C:511:HOH:O	2.10	0.51
1:B:115:LYS:HA	8:B:580:HOH:O	2.09	0.51
1:C:226:LEU:CD1	1:C:283:LEU:HD23	2.41	0.51
1:A:364:MET:HG3	1:A:371:VAL:CG1	2.41	0.50
1:A:478:PRO:HD2	8:A:605:HOH:O	2.09	0.50
1:C:101:LEU:HD21	1:C:132:GLU:CD	2.32	0.50
1:A:72:LYS:HB3	1:A:73:PHE:O	2.12	0.50
1:C:102:GLU:HB3	1:C:126:TYR:OH	2.11	0.50
1:A:13:ASN:ND2	1:A:172:LEU:HA	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:GLU:HG2	1:C:473[B]:MET:HG3	1.92	0.50
1:C:226:LEU:HD12	1:C:283:LEU:CD2	2.40	0.50
1:A:144:PRO:HA	1:A:147:PHE:CE2	2.47	0.50
1:A:191:ILE:HG13	1:A:499:PRO:HG3	1.93	0.49
1:B:235:ASN:HD22	1:B:237:ALA:H	1.58	0.49
1:B:219:GLY:HA2	1:B:472:MET:HE1	1.94	0.49
1:A:10:TRP:HE1	1:A:26:GLN:HE21	1.59	0.49
1:B:54:TRP:HB3	1:B:65:PHE:CD1	2.47	0.49
1:C:14:VAL:HG12	1:C:17:LEU:HD23	1.95	0.49
1:C:16:PRO:O	1:C:17:LEU:HB2	2.13	0.49
1:A:181:ASN:HD22	1:A:184:TYR:HB2	1.76	0.49
1:A:255:THR:HG22	1:A:266:ARG:CZ	2.43	0.49
1:B:350:ASP:OD1	1:B:352:LEU:HB3	2.13	0.49
1:B:100:TRP:CH2	1:B:101:LEU:HG	2.47	0.49
1:B:20:HIS:CE1	1:B:87:ASN:HD22	2.31	0.49
1:A:343[B]:GLU:HG3	1:A:391:GLY:H	1.78	0.49
1:C:8:THR:HG22	1:C:9:ALA:H	1.77	0.49
1:A:8:THR:HG22	1:A:9:ALA:N	2.25	0.48
1:C:17:LEU:HB3	1:C:159:PRO:HB3	1.95	0.48
1:B:19:PRO:HG3	1:B:142:ILE:HB	1.94	0.48
1:C:253:LEU:HD22	1:C:392:MET:HG2	1.95	0.48
1:B:278:LEU:HD23	1:B:278:LEU:O	2.12	0.48
1:A:164:PRO:HG3	1:A:184:TYR:CZ	2.48	0.48
1:C:278:LEU:HD21	1:C:356:MET:HG2	1.94	0.48
1:C:382:TYR:CE2	1:C:416:HIS:CE1	3.01	0.48
1:B:18:ASN:CG	1:B:21:LEU:HD23	2.33	0.48
1:A:74:SER:HB2	1:A:161:GLY:O	2.14	0.48
1:C:164:PRO:HD3	1:C:184:TYR:CE1	2.49	0.48
1:C:279:ILE:HA	1:C:283:LEU:HD12	1.96	0.48
1:A:313:GLN:HG3	8:A:604:HOH:O	2.11	0.48
1:C:209:PHE:HA	1:C:214:ILE:HG13	1.95	0.48
1:A:311:ASP:OD2	1:A:314[B]:LYS:HG3	2.13	0.47
1:B:276[A]:LYS:HD2	8:B:622:HOH:O	2.14	0.47
1:C:8:THR:HG23	1:C:216:LEU:O	2.14	0.47
1:C:283:LEU:CD2	1:C:352:LEU:HD11	2.44	0.47
1:A:14[A]:VAL:CG1	1:A:29:ALA:CB	2.91	0.47
1:B:27:MET:HE2	1:B:136:PRO:HG2	1.96	0.47
1:B:217:LEU:CD1	1:B:224:LEU:HD22	2.44	0.47
1:C:428:LYS:O	1:C:428:LYS:HD2	2.14	0.47
1:C:92:LEU:C	1:C:94:ASN:H	2.18	0.47
1:A:339:PRO:HB2	1:A:341[B]:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:HD21	1:C:473[A]:MET:CE	2.44	0.47
1:A:93:ASP:O	3:A:507:ACT:CH3	2.62	0.47
1:C:227:ASP:HB3	1:C:284:TYR:OH	2.14	0.47
1:C:226:LEU:CD1	1:C:283:LEU:CD2	2.92	0.47
1:C:293:LEU:H	3:C:504:ACT:C	2.27	0.47
1:A:349:THR:OG1	7:A:513:GOL:H12	2.15	0.47
1:B:364:MET:HG3	1:B:371:VAL:CG1	2.44	0.47
1:C:103:LEU:HB2	1:C:132:GLU:OE2	2.15	0.47
1:C:316:LYS:HG2	1:C:333:ARG:NH1	2.30	0.47
1:C:354:LYS:O	1:C:358[A]:GLU:HG3	2.15	0.47
1:B:258:ALA:HA	1:B:261:ASN:OD1	2.15	0.46
1:C:66:THR:C	1:C:67:LEU:O	2.53	0.46
1:A:146:GLN:HE21	1:A:158:ALA:H	1.63	0.46
1:C:146:GLN:OE1	1:C:157:LYS:HB2	2.14	0.46
1:C:40:TYR:HB3	1:C:488:ILE:HD11	1.97	0.46
1:A:27:MET:CE	1:A:136:PRO:HG2	2.45	0.46
1:B:320:GLU:OE2	1:B:325:THR:HG22	2.14	0.46
1:B:473[A]:MET:CE	8:B:569:HOH:O	2.64	0.46
7:A:514:GOL:H31	1:B:42:ALA:N	2.20	0.46
1:A:316:LYS:HE2	1:A:333:ARG:NH1	2.11	0.46
1:C:278:LEU:HD11	1:C:356:MET:HG2	1.98	0.46
1:C:93:ASP:OD2	1:C:151:GLU:OE1	2.34	0.46
1:C:420:GLN:HA	1:C:420:GLN:NE2	2.30	0.46
1:C:225:PRO:HB2	1:C:227:ASP:OD1	2.16	0.46
1:B:226:LEU:HD12	1:B:283:LEU:HA	1.96	0.46
1:B:336:ASN:HB3	1:C:457:ARG:HH12	1.80	0.46
1:C:6:ILE:O	1:C:194:ILE:HA	2.15	0.46
1:B:127:TYR:CD2	1:B:128:PRO:HD3	2.51	0.45
1:B:373:LEU:HD22	7:B:515:GOL:H31	1.97	0.45
1:B:373:LEU:C	1:B:374:ILE:HG12	2.36	0.45
1:C:221:GLU:OE1	1:C:287[A]:GLN:CG	2.65	0.45
1:A:331:ASP:CB	1:A:365:ARG:HH11	2.29	0.45
1:B:97[B]:ARG:HH11	1:B:386:ARG:HH11	1.57	0.45
1:C:253:LEU:CD2	1:C:392:MET:HG2	2.46	0.45
1:A:386:ARG:CA	1:A:415:SER:OG	2.64	0.45
1:A:93:ASP:O	3:A:507:ACT:H1	2.16	0.45
1:B:218:TYR:H	3:B:507:ACT:C	2.30	0.45
1:C:11:PRO:HA	1:C:199:ILE:O	2.17	0.45
1:C:396[A]:ARG:CZ	3:C:506:ACT:H1	2.43	0.45
1:A:127:TYR:CG	1:A:128:PRO:HD3	2.51	0.45
1:C:226:LEU:HD13	1:C:283:LEU:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96[B]:GLN:HB2	3:A:507:ACT:O	2.17	0.45
7:A:514:GOL:H31	1:B:42:ALA:HB3	1.99	0.45
1:A:254:ASN:C	1:A:254:ASN:HD22	2.21	0.45
1:B:191:ILE:HG21	1:B:194:ILE:CD1	2.47	0.45
1:A:377[A]:GLU:H	1:A:377[A]:GLU:CD	2.20	0.44
1:B:27:MET:CE	1:B:136:PRO:HG2	2.47	0.44
1:C:283:LEU:HD22	1:C:352:LEU:CD1	2.47	0.44
1:C:399:GLY:N	1:C:403:ASP:OD2	2.51	0.44
1:C:342:ILE:O	1:C:371:VAL:HA	2.17	0.44
1:C:6:ILE:HD11	1:C:191:ILE:HG13	2.00	0.44
1:B:89:ARG:NH2	1:B:150:HIS:HB3	2.33	0.44
1:C:14:VAL:HG13	1:C:29:ALA:CB	2.48	0.44
1:C:49:TRP:C	1:C:51:ALA:H	2.20	0.44
1:C:68:ARG:HG3	1:C:71:VAL:HG23	1.99	0.44
1:A:289:VAL:N	3:A:506:ACT:OXT	2.49	0.44
1:B:373:LEU:HB2	7:B:515:GOL:H11	2.00	0.44
1:B:306:LYS:HA	1:B:307:PRO:HD2	1.91	0.44
1:C:68:ARG:CB	1:C:69:ASP:HA	2.46	0.44
1:C:298:VAL:HG13	1:C:299:PRO:HD2	2.00	0.44
1:C:206:ALA:HB1	1:C:228:THR:HG21	1.99	0.44
1:C:459:HIS:ND1	3:C:504:ACT:OXT	2.39	0.44
1:A:20:HIS:CE1	1:A:140:ARG:O	2.70	0.44
1:A:227:ASP:HB3	1:A:284:TYR:CE2	2.53	0.44
1:A:398:TRP:CE2	6:A:511:HCT:H5A	2.53	0.44
1:B:226:LEU:HD22	3:B:504:ACT:O	2.18	0.44
1:A:278:LEU:HD23	1:A:278:LEU:C	2.38	0.43
1:A:415:SER:O	1:A:416:HIS:HD2	2.01	0.43
1:B:217:LEU:HD23	3:B:507:ACT:H2	1.98	0.43
1:C:131:GLN:HG2	1:C:131:GLN:H	1.16	0.43
1:A:142:ILE:HG23	1:A:142:ILE:O	2.17	0.43
1:B:253:LEU:HB2	1:B:463:VAL:O	2.18	0.43
1:C:10:TRP:CD2	1:C:11:PRO:HD2	2.53	0.43
1:C:398:TRP:HZ2	1:C:416:HIS:CD2	2.37	0.43
1:A:64:THR:HA	1:A:118:LEU:O	2.18	0.43
1:A:360:ILE:HG23	1:A:364:MET:HE1	2.00	0.43
1:B:20:HIS:CD2	1:B:152:THR:OG1	2.64	0.43
1:C:88:PHE:CB	1:C:110:VAL:HG21	2.48	0.43
1:C:458:LEU:HD23	1:C:458:LEU:HA	1.80	0.43
1:C:28:PHE:HB2	1:C:492:ILE:HG12	2.00	0.43
1:A:95:ARG:HH11	1:A:95:ARG:CB	2.29	0.43
1:B:235:ASN:HD22	1:B:236:PRO:N	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444[A]:GLU:HG3	1:C:447:ARG:HH21	1.83	0.43
1:B:284:TYR:N	1:B:285:GLY:HA3	2.34	0.43
1:B:72[B]:LYS:HD3	1:B:78:PRO:HA	2.00	0.43
1:C:218:TYR:CD2	1:C:492:ILE:HD12	2.54	0.43
1:B:35:GLU:HA	1:B:36:PRO:HD3	1.89	0.43
1:C:411:MET:HG2	1:C:418:ASP:HB3	2.01	0.43
1:B:192[B]:LYS:CE	8:B:597:HOH:O	2.67	0.43
1:C:272:ALA:HB2	1:C:367[B]:ILE:HD13	2.01	0.43
1:C:272:ALA:O	1:C:363:ASP:HB3	2.19	0.43
1:B:9:ALA:O	3:B:507:ACT:CH3	2.67	0.42
1:A:158:ALA:O	1:A:160:ILE:N	2.50	0.42
1:B:174:GLN:O	1:B:175:TYR:HB3	2.19	0.42
1:B:361:GLN:HE22	7:B:515:GOL:H31	1.84	0.42
1:C:127:TYR:CG	1:C:128:PRO:HD3	2.54	0.42
1:A:224:LEU:HD21	1:A:229:PHE:HB2	2.01	0.42
1:A:20:HIS:CE1	1:A:87:ASN:HD22	2.35	0.42
1:B:131:GLN:HG2	1:B:131:GLN:H	1.60	0.42
1:B:219:GLY:C	1:B:472:MET:CE	2.88	0.42
1:C:12:VAL:HG13	1:C:13:ASN:O	2.20	0.42
1:C:408:LEU:HD13	1:C:454:ILE:HG21	2.00	0.42
1:A:89:ARG:HH22	1:A:150:HIS:HB3	1.85	0.42
1:B:274:ASN:OD1	1:B:277:SER:CB	2.56	0.42
1:A:374:ILE:HG22	1:A:376:GLU:HG3	2.00	0.42
1:A:54:TRP:HB3	1:A:65:PHE:CD1	2.54	0.42
1:C:101:LEU:HD21	1:C:132:GLU:CG	2.50	0.42
1:B:226:LEU:HD23	1:B:226:LEU:HA	1.93	0.42
1:A:221:GLU:HG3	1:A:470:ILE:HB	2.01	0.42
1:B:12:VAL:HG13	1:B:13:ASN:O	2.19	0.42
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.83	0.42
1:C:217:LEU:HD23	1:C:217:LEU:HA	1.92	0.42
1:A:384:ARG:HA	1:A:387:ASP:HB2	2.02	0.42
1:A:338:GLN:HA	1:A:339:PRO:HD3	1.95	0.41
1:A:395:HIS:CE1	8:A:603:HOH:O	2.72	0.41
1:B:275:LYS:HD2	1:B:289:VAL:HG13	2.02	0.41
1:C:17:LEU:HD22	1:C:17:LEU:HA	1.73	0.41
1:B:13:ASN:ND2	1:B:173:ASN:H	2.16	0.41
1:B:181:ASN:ND2	1:B:183:ASN:H	2.19	0.41
1:C:409:SER:HB2	1:C:439:LEU:HD21	2.02	0.41
1:C:356:MET:CE	1:C:467:ILE:HG21	2.50	0.41
1:A:235:ASN:HA	1:A:236:PRO:HD3	1.94	0.41
1:A:408:LEU:HD13	1:A:454:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:GLY:CA	1:B:472:MET:HE1	2.50	0.41
1:C:419:PHE:HB3	8:C:535:HOH:O	2.20	0.41
1:A:292:THR:O	1:A:293:LEU:C	2.57	0.41
1:B:465:LEU:HD23	1:B:465:LEU:C	2.41	0.41
1:B:274:ASN:HB2	1:B:310:TYR:CD1	2.55	0.41
1:C:20:HIS:CD2	1:C:152:THR:HG21	2.55	0.41
1:C:411:MET:HG2	1:C:418:ASP:CB	2.50	0.41
1:A:438:VAL:HG23	1:A:450:LEU:HB2	2.03	0.41
1:A:181:ASN:ND2	1:A:184:TYR:HB2	2.36	0.41
1:C:101:LEU:HD22	1:C:132:GLU:OE2	2.21	0.41
1:C:180:ARG:NH1	1:C:189:PRO:O	2.54	0.41
1:C:240:THR:HG22	1:C:475:VAL:HG22	2.02	0.41
1:C:434:GLU:OE1	1:C:453:ASP:OD2	2.39	0.41
1:C:68:ARG:HA	1:C:68:ARG:HD3	1.45	0.41
1:A:483:ILE:HA	1:A:484:PRO:HD3	1.87	0.41
1:B:346:PHE:HB3	1:B:394:PHE:HD1	1.86	0.41
1:B:408:LEU:HD12	1:B:451:TYR:HE2	1.86	0.41
1:C:6:ILE:CD1	1:C:191:ILE:HG13	2.50	0.41
1:C:283:LEU:HD21	1:C:352:LEU:HD11	2.00	0.41
1:A:342:ILE:O	1:A:371:VAL:HA	2.21	0.41
1:A:72:LYS:HG2	8:A:592:HOH:O	2.21	0.41
1:C:395:HIS:O	1:C:396[B]:ARG:HG3	2.21	0.41
1:C:396[A]:ARG:NE	3:C:506:ACT:H3	2.35	0.41
1:B:240:THR:HG22	1:B:475:VAL:HG22	2.03	0.40
1:B:217:LEU:HA	3:B:507:ACT:CH3	2.51	0.40
1:C:38:VAL:HG21	1:C:46:VAL:CG1	2.50	0.40
1:A:331:ASP:HB3	1:A:365:ARG:NH1	2.35	0.40
1:B:27:MET:HG3	8:B:624:HOH:O	2.21	0.40
1:A:175:TYR:HA	1:A:196:PHE:O	2.22	0.40
1:B:165:TRP:HH2	1:B:191:ILE:HB	1.87	0.40
1:C:221:GLU:HA	1:C:473[B]:MET:SD	2.62	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	511/502 (102%)	473 (93%)	33 (6%)	5 (1%)	18	32
1	B	510/502 (102%)	478 (94%)	30 (6%)	2 (0%)	38	59
1	C	505/502 (101%)	467 (92%)	31 (6%)	7 (1%)	13	23
All	All	1526/1506 (101%)	1418 (93%)	94 (6%)	14 (1%)	20	36

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	67	LEU
1	A	74	SER
1	C	59	ASP
1	C	282	ALA
1	A	113	LEU
1	B	286	THR
1	C	17	LEU
1	C	95	ARG
1	A	347	ILE
1	B	340	LEU
1	A	145	SER
1	C	220	ASN
1	C	415	SER
1	A	493	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	435/425 (102%)	392 (90%)	43 (10%)	9	17
1	B	440/425 (104%)	404 (92%)	36 (8%)	13	25
1	C	432/425 (102%)	381 (88%)	51 (12%)	6	11
All	All	1307/1275 (102%)	1177 (90%)	130 (10%)	9	17

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	23	THR
1	A	38	VAL
1	A	46	VAL
1	A	53	SER
1	A	58	GLU
1	A	64	THR
1	A	86	GLU
1	A	94	ASN
1	A	95	ARG
1	A	101	LEU
1	A	103	LEU
1	A	120	ILE
1	A	121	THR
1	A	123	LYS
1	A	131[A]	GLN
1	A	131[B]	GLN
1	A	145	SER
1	A	167	LEU
1	A	171	LYS
1	A	172	LEU
1	A	173	ASN
1	A	181	ASN
1	A	182	GLU
1	A	216	LEU
1	A	221	GLU
1	A	224	LEU
1	A	242	LEU
1	A	248	THR
1	A	250	MET
1	A	254	ASN
1	A	316	LYS
1	A	319	LEU
1	A	325	THR
1	A	331	ASP
1	A	373	LEU
1	A	387	ASP
1	A	416	HIS
1	A	438	VAL
1	A	439	LEU
1	A	452	ARG
1	A	479	GLU

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Mol	Chain	Res	Type
1	A	482	ASN
1	B	4	ASP
1	B	7	THR
1	B	12	VAL
1	B	38	VAL
1	B	71	VAL
1	B	101	LEU
1	B	103	LEU
1	B	111	LYS
1	B	131	GLN
1	B	150	HIS
1	B	167	LEU
1	B	181	ASN
1	B	216	LEU
1	B	224	LEU
1	B	235	ASN
1	B	250	MET
1	B	253	LEU
1	B	283	LEU
1	B	288[A]	GLN
1	B	288[B]	GLN
1	B	309[A]	GLN
1	B	309[B]	GLN
1	B	319	LEU
1	B	345	SER
1	B	355	SER
1	B	364	MET
1	B	365	ARG
1	B	374	ILE
1	B	380	SER
1	B	392	MET
1	B	410	SER
1	B	439	LEU
1	B	450	LEU
1	B	473[A]	MET
1	B	473[B]	MET
1	B	490	THR
1	C	8	THR
1	C	12	VAL
1	C	17	LEU
1	C	27	MET
1	C	43	ASP

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Mol	Chain	Res	Type
1	C	46	VAL
1	C	53	SER
1	C	58	GLU
1	C	64	THR
1	C	68	ARG
1	C	77	GLU
1	C	95	ARG
1	C	96	GLN
1	C	101	LEU
1	C	103	LEU
1	C	116	THR
1	C	123	LYS
1	C	130	LEU
1	C	131	GLN
1	C	148	LYS
1	C	167	LEU
1	C	169	GLU
1	C	179	VAL
1	C	182	GLU
1	C	213	ASP
1	C	216	LEU
1	C	224	LEU
1	C	246	ILE
1	C	249	VAL
1	C	250	MET
1	C	276	LYS
1	C	303	LEU
1	C	306	LYS
1	C	320[A]	GLU
1	C	320[B]	GLU
1	C	341	ARG
1	C	371	VAL
1	C	373	LEU
1	C	380	SER
1	C	387	ASP
1	C	396[A]	ARG
1	C	396[B]	ARG
1	C	438	VAL
1	C	439	LEU
1	C	441	THR
1	C	450	LEU
1	C	452	ARG

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Mol	Chain	Res	Type
1	C	473[A]	MET
1	C	473[B]	MET
1	C	490	THR
1	C	498	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	26	GLN
1	A	87	ASN
1	A	94	ASN
1	A	106	GLN
1	A	146	GLN
1	A	181	ASN
1	A	244	GLN
1	A	254	ASN
1	A	338	GLN
1	A	405	HIS
1	A	420	GLN
1	A	442	HIS
1	A	446	GLN
1	A	459	HIS
1	A	496	GLN
1	B	13	ASN
1	B	20	HIS
1	B	26	GLN
1	B	87	ASN
1	B	94	ASN
1	B	146	GLN
1	B	150	HIS
1	B	174	GLN
1	B	181	ASN
1	B	235	ASN
1	B	241	GLN
1	B	338	GLN
1	B	420	GLN
1	B	448	GLN
1	C	13	ASN
1	C	20	HIS
1	C	26	GLN
1	C	56	HIS

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Mol	Chain	Res	Type
1	C	87	ASN
1	C	181	ASN
1	C	338	GLN
1	C	416	HIS
1	C	420	GLN
1	C	482	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 10 are monoatomic - leaving 23 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACT	A	504	-	1,3,3	1.38	0	0,3,3	0.00	-
3	ACT	A	505	-	1,3,3	1.87	0	0,3,3	0.00	-
3	ACT	A	506	-	1,3,3	2.06	1 (100%)	0,3,3	0.00	-
3	ACT	A	507	-	1,3,3	2.14	1 (100%)	0,3,3	0.00	-
4	SO4	A	508	-	4,4,4	0.16	0	6,6,6	0.36	0
6	HCT	A	511	2	3,12,12	2.82	1 (33%)	4,15,15	5.34	3 (75%)
7	GOL	A	512	-	5,5,5	0.23	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	A	513	-	5,5,5	0.43	0	5,5,5	0.56	0
7	GOL	A	514	-	5,5,5	0.37	0	5,5,5	0.39	0
7	GOL	A	515	-	5,5,5	0.39	0	5,5,5	0.38	0
3	ACT	B	504	-	1,3,3	2.14	1 (100%)	0,3,3	0.00	-
3	ACT	B	505	-	1,3,3	2.28	1 (100%)	0,3,3	0.00	-
3	ACT	B	506	-	1,3,3	2.84	1 (100%)	0,3,3	0.00	-
3	ACT	B	507	-	1,3,3	0.20	0	0,3,3	0.00	-
6	HCT	B	511	2	3,12,12	4.26	1 (33%)	4,15,15	3.22	3 (75%)
7	GOL	B	512	-	5,5,5	0.38	0	5,5,5	0.48	0
7	GOL	B	513	-	5,5,5	0.29	0	5,5,5	0.78	0
7	GOL	B	514	-	5,5,5	0.32	0	5,5,5	0.29	0
7	GOL	B	515	-	5,5,5	0.56	0	5,5,5	0.92	0
3	ACT	C	504	-	1,3,3	6.99	1 (100%)	0,3,3	0.00	-
3	ACT	C	505	-	1,3,3	1.49	0	0,3,3	0.00	-
3	ACT	C	506	-	1,3,3	2.48	1 (100%)	0,3,3	0.00	-
6	HCT	C	509	2	3,12,12	2.92	1 (33%)	4,15,15	4.57	2 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	A	504	-	-	0/0/0/0	0/0/0/0
3	ACT	A	505	-	-	0/0/0/0	0/0/0/0
3	ACT	A	506	-	-	0/0/0/0	0/0/0/0
3	ACT	A	507	-	-	0/0/0/0	0/0/0/0
4	SO4	A	508	-	-	0/0/0/0	0/0/0/0
6	HCT	A	511	2	-	0/5/13/13	0/0/0/0
7	GOL	A	512	-	-	0/4/4/4	0/0/0/0
7	GOL	A	513	-	-	0/4/4/4	0/0/0/0
7	GOL	A	514	-	-	0/4/4/4	0/0/0/0
7	GOL	A	515	-	-	0/4/4/4	0/0/0/0
3	ACT	B	504	-	-	0/0/0/0	0/0/0/0
3	ACT	B	505	-	-	0/0/0/0	0/0/0/0
3	ACT	B	506	-	-	0/0/0/0	0/0/0/0
3	ACT	B	507	-	-	0/0/0/0	0/0/0/0
6	HCT	B	511	2	-	0/5/13/13	0/0/0/0
7	GOL	B	512	-	-	0/4/4/4	0/0/0/0
7	GOL	B	513	-	-	0/4/4/4	0/0/0/0
7	GOL	B	514	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	515	-	-	0/4/4/4	0/0/0/0
3	ACT	C	504	-	-	0/0/0/0	0/0/0/0
3	ACT	C	505	-	-	0/0/0/0	0/0/0/0
3	ACT	C	506	-	-	0/0/0/0	0/0/0/0
6	HCT	C	509	2	-	0/5/13/13	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	506	ACT	CH3-C	2.06	1.51	1.48
3	B	504	ACT	CH3-C	2.14	1.51	1.48
3	A	507	ACT	CH3-C	2.14	1.51	1.48
3	B	505	ACT	CH3-C	2.28	1.51	1.48
3	C	506	ACT	CH3-C	2.48	1.51	1.48
3	B	506	ACT	CH3-C	2.84	1.52	1.48
6	A	511	HCT	C2-C3	4.71	1.61	1.54
6	C	509	HCT	C2-C3	5.01	1.61	1.54
3	C	504	ACT	CH3-C	6.99	1.57	1.48
6	B	511	HCT	C2-C3	7.16	1.64	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	511	HCT	C4-C3-C7	-8.83	98.44	112.70
6	C	509	HCT	C4-C3-C7	-6.90	101.56	112.70
6	B	511	HCT	C4-C3-C7	-2.60	108.50	112.70
6	A	511	HCT	C5-C4-C3	-2.57	108.44	113.39
6	B	511	HCT	C2-C3-C7	2.85	116.97	111.08
6	B	511	HCT	C5-C4-C3	5.10	123.19	113.39
6	A	511	HCT	C2-C3-C7	5.42	122.26	111.08
6	C	509	HCT	C2-C3-C7	5.67	122.78	111.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	506	ACT	2	0
3	A	507	ACT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	511	HCT	1	0
7	A	512	GOL	1	0
7	A	513	GOL	4	0
7	A	514	GOL	10	0
3	B	504	ACT	1	0
3	B	507	ACT	15	0
7	B	513	GOL	4	0
7	B	515	GOL	5	0
3	C	504	ACT	3	0
3	C	506	ACT	15	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	498/502 (99%)	-0.26	6 (1%) 79 80	28, 46, 66, 76	0
1	B	497/502 (99%)	-0.29	5 (1%) 82 83	30, 44, 63, 83	1 (0%)
1	C	496/502 (98%)	0.04	23 (4%) 33 35	32, 60, 87, 99	1 (0%)
All	All	1491/1506 (99%)	-0.17	34 (2%) 61 63	28, 49, 79, 99	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	ASN	4.3
1	A	3	PRO	3.9
1	C	157	LYS	3.4
1	A	2	ALA	3.3
1	C	499	PRO	3.3
1	C	188	LYS	3.2
1	C	150	HIS	3.2
1	A	183	ASN	3.1
1	C	281	ASN	2.9
1	C	149	ASN	2.8
1	B	328	ALA	2.7
1	C	52	LYS	2.6
1	C	172	LEU	2.6
1	C	192	LYS	2.5
1	C	148	LYS	2.5
1	C	162	THR	2.5
1	C	161	GLY	2.4
1	C	171	LYS	2.4
1	C	175	TYR	2.4
1	C	329	GLY	2.3
1	C	498	LYS	2.3
1	C	67	LEU	2.3
1	B	58[A]	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	68	ARG	2.3
1	B	120	ILE	2.3
1	C	194	ILE	2.2
1	A	387	ASP	2.2
1	B	96[A]	GLN	2.2
1	C	96	GLN	2.2
1	C	58	GLU	2.2
1	A	414	PRO	2.1
1	A	149	ASN	2.1
1	C	408	LEU	2.0
1	C	69	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	B	515	6/6	0.62	0.53	15.82	29,40,42,42	6
3	ACT	B	504	4/4	0.58	0.54	7.61	41,41,41,42	4
7	GOL	A	512	6/6	0.66	0.46	7.00	57,59,61,63	6
7	GOL	A	515	6/6	0.58	0.45	6.53	51,54,55,55	6
7	GOL	B	513	6/6	0.78	0.38	6.47	28,30,31,33	6
3	ACT	C	506	4/4	0.72	0.45	6.27	34,34,35,35	4
7	GOL	A	514	6/6	0.79	0.31	5.66	39,42,44,45	6
3	ACT	A	506	4/4	0.79	0.37	3.98	57,58,58,58	4
3	ACT	B	506	4/4	0.48	0.52	3.93	41,43,43,43	4
3	ACT	A	504	4/4	0.93	0.14	3.50	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACT	C	504	4/4	0.93	0.19	3.12	37,38,38,39	0
3	ACT	A	507	4/4	0.73	0.43	3.00	48,49,49,50	4
3	ACT	B	507	4/4	0.87	0.33	2.89	36,37,37,37	4
7	GOL	A	513	6/6	0.89	0.24	0.89	45,49,50,51	6
6	HCT	A	511	13/13	0.94	0.15	0.55	33,53,61,61	0
6	HCT	C	509	13/13	0.90	0.16	0.47	48,58,65,67	0
6	HCT	B	511	13/13	0.95	0.11	-0.08	35,47,52,53	0
5	CL	B	509	1/1	0.98	0.09	-0.94	40,40,40,40	0
7	GOL	B	514	6/6	0.91	0.16	-1.56	51,52,53,55	6
5	CL	A	510	1/1	0.84	0.09	-	90,90,90,90	0
2	NI	B	503	1/1	0.98	0.02	-	53,53,53,53	0
2	NI	C	503	1/1	0.96	0.05	-	66,66,66,66	0
4	SO4	A	508	5/5	0.86	0.16	-	47,48,52,52	5
3	ACT	C	505	4/4	0.89	0.16	-	40,40,40,40	4
5	CL	B	510	1/1	0.88	0.18	-	50,50,50,50	1
7	GOL	B	512	6/6	0.83	0.26	-	46,49,50,51	6
3	ACT	B	505	4/4	0.96	0.21	-	65,66,66,66	0
5	CL	A	509	1/1	0.96	0.07	-	61,61,61,61	0
5	CL	B	508	1/1	0.92	0.22	-	44,44,44,44	1
5	CL	C	507	1/1	0.98	0.07	-	57,57,57,57	0
2	NI	A	503	1/1	0.98	0.06	-	78,78,78,78	0
5	CL	C	508	1/1	0.98	0.07	-	58,58,58,58	0
3	ACT	A	505	4/4	0.74	0.18	-	45,45,45,46	4

## 6.5 Other polymers [i](#)

There are no such residues in this entry.